Ion Stopping in WDM

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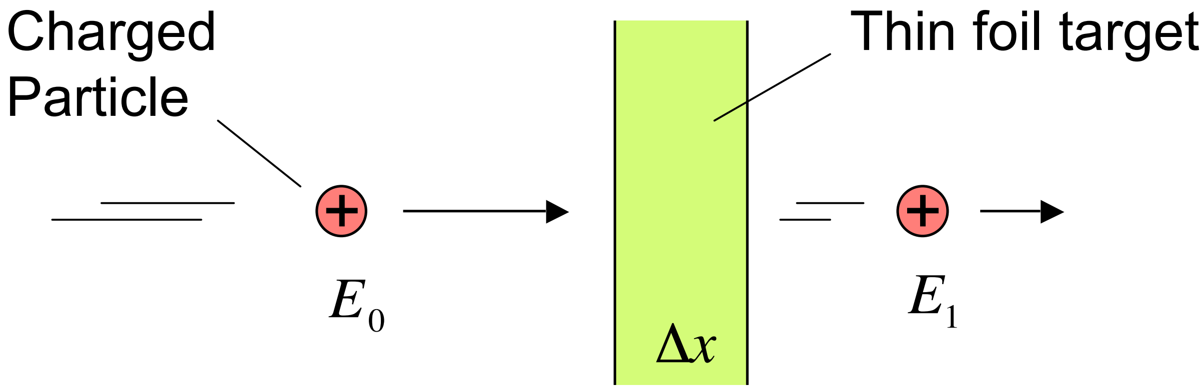
Definition of stopping power (stopping force)



$$-\left.\frac{dE}{dx}\right|_{E=E_1} = -\lim_{\Delta x \to 0} (E_1 - E_0)/\Delta x$$

- In practice, the "averaged" stopping power is measured by:

$$-\left.\frac{dE}{dx}\right|_{E=E_0-\Delta E/2} \cong -\frac{\Delta E}{\Delta x} = \frac{E_0 - E_1}{\Delta x}, \quad \Delta E < 0.2 E_0$$

Energetic charged particles lose their kinetic energy in matter by collisions and radiations.

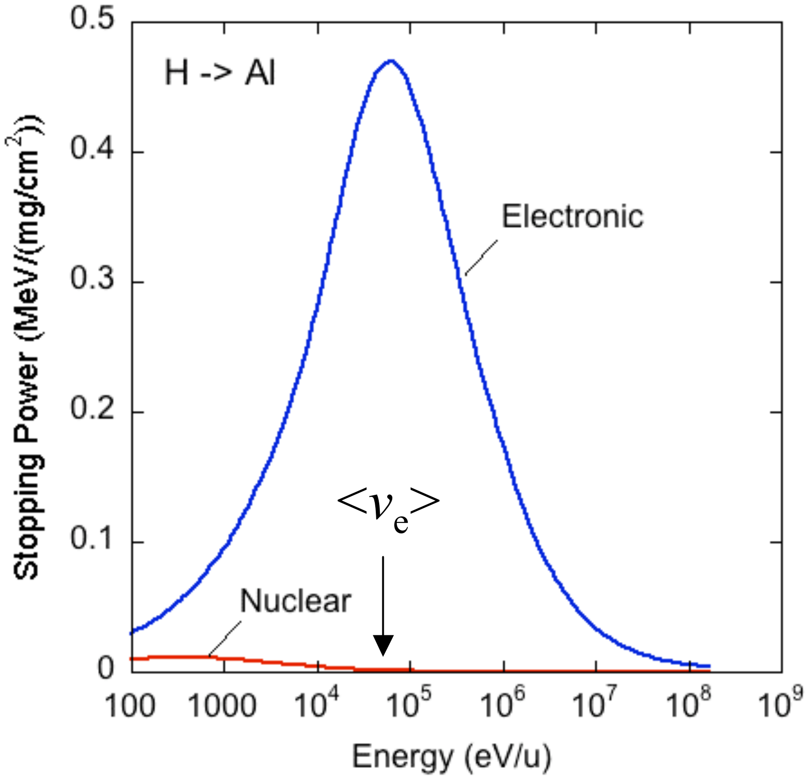
- Elastic collision: **nuclear stopping power**
  - Particular for heavy particles with low velocities around 1 keV/u.
  - Projectile kinetic energy is transferred to recoiled atoms without any excitation of electronic systems.

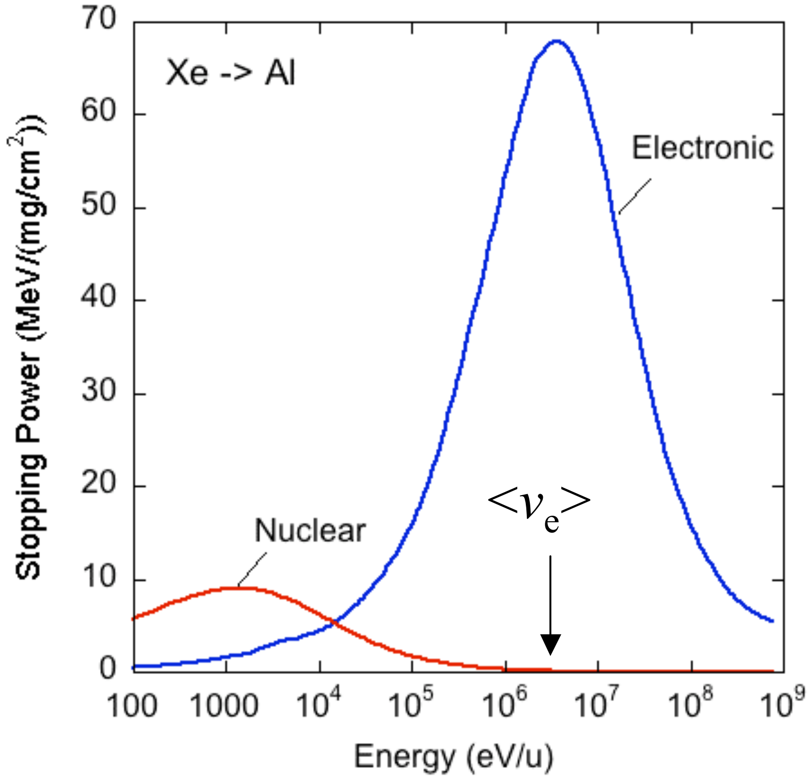
- Inelastic collision: **electronic stopping power**
  - A dominant stopping process for projectiles above 1 keV/u.

  1. Electronic excitation and ionization of the target.
  2. Projectile excitation and ionization.
  3. Electron capture.

- Electromagnetic radiation
  - Particular for light particles at extremely high velocities (β~1).
    (> 1 MeV for electron)
  - Bremsstrahlung (breaking radiation) is dominant.

Stopping power strongly depends on projectile "velocity".





- Electronic stopping power has a peak when the projectile velocity is almost equal to the mean velocities of target electrons $<v_e>$.

$$\boxed{< v_e >= Z_2^{2/3} v_B}$$

v_B : Bohr velocity = 2.2 x 10^8 cm/s

The beam energy deposition profile is determined by the dE/dx curve.

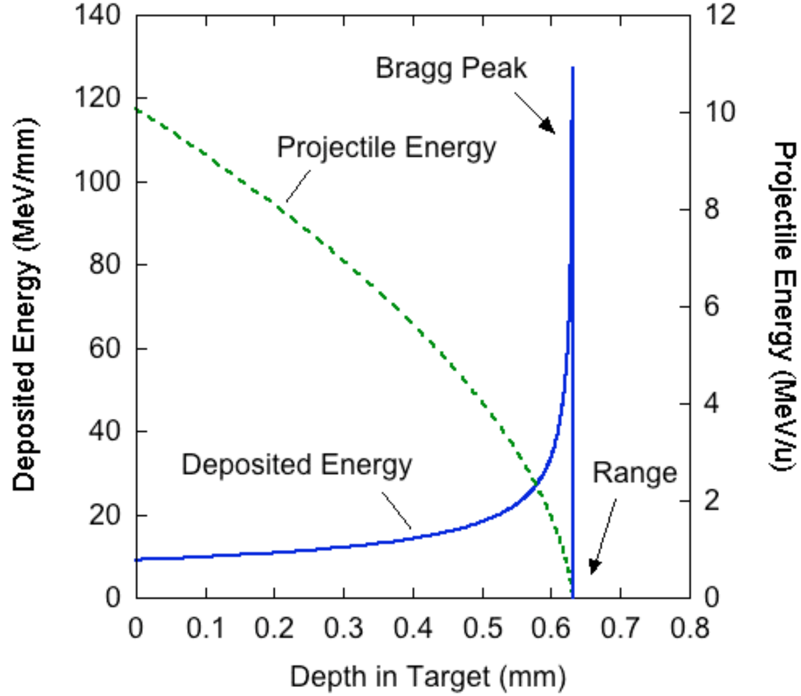
Range:

$$R = \int_{E_0}^{0} \frac{1}{dE/dx} dE'$$

Energy deposition profile:

$$\Delta e(x) \approx \frac{j\tau}{q} \frac{dE}{dx}(E(x))$$

$$x(E) = \int_{E_0}^{E} \frac{1}{dE/dx} dE'$$



j: beam current density, τ: beam pulse length, q: projectile charge

- The range value has an uncertainty due to probabilistic behaviors of projectiles in the target (range straggling).
- Energy deposition processes become much more complex when changes in target properties (n, T, etc.) is not negligible.

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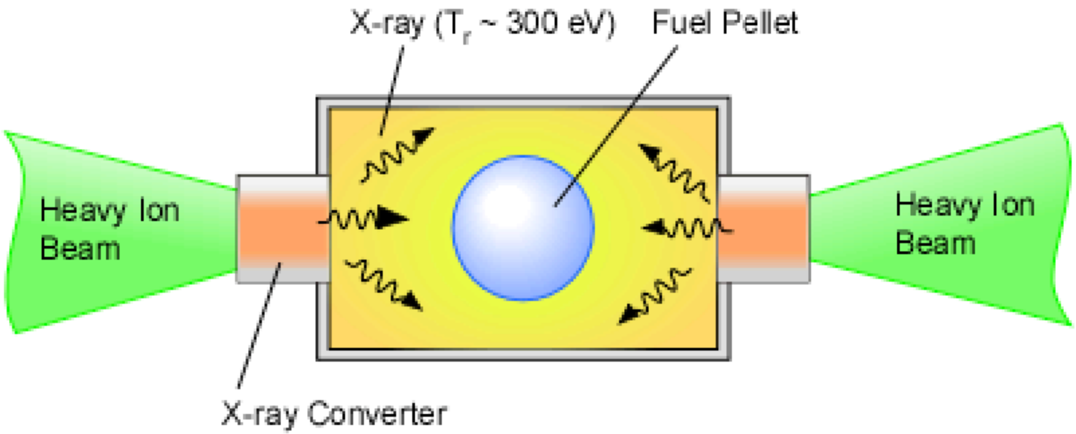
Beam-energy deposition profile is very important in HIF target design.



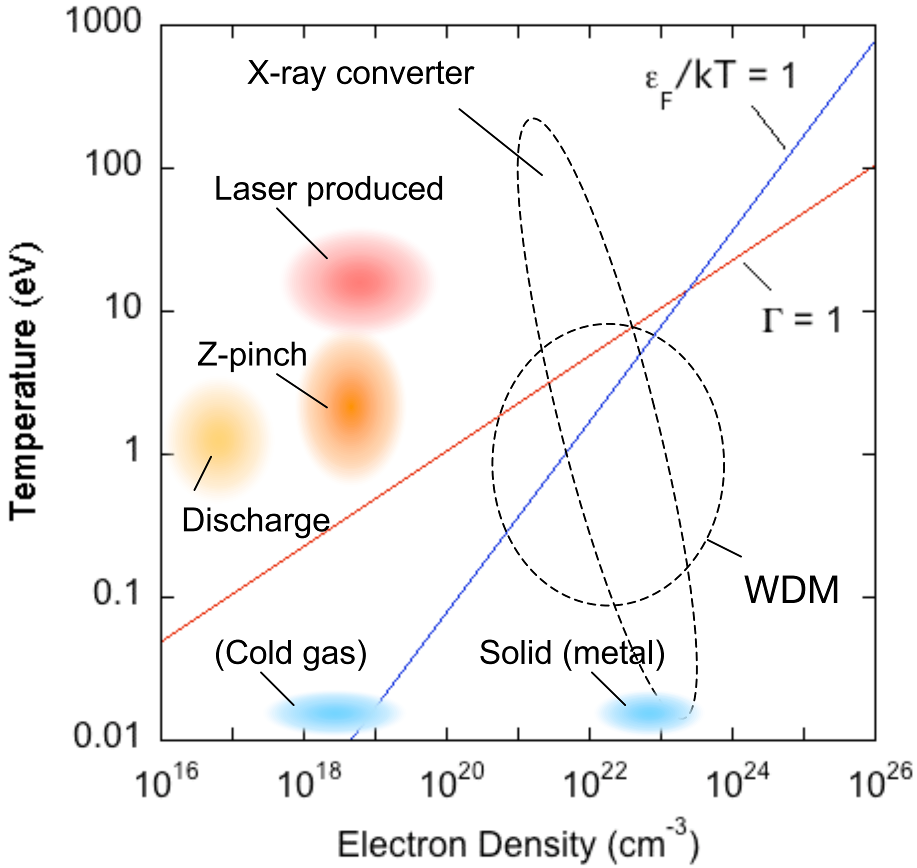
E ~ 10 GeV
I ~ 10 kA
τ ~ 20 ns

- The overall gain of the HIF target strongly depends on the uniformity and time variation of the black body radiation.
- The density and temperature of the X-ray radiator dynamically change within a short period of beam irradiation (~20 ns).

⇓

- To optimize the HIF target design with hydrodynamic simulations including ion stopping processes, reliable data of stopping power over a wide density-temperature range is required.

Stopping power data is available only for limited density-temperature ranges.



- There are reliable databases for stopping power of cold matter. (SRIM, NIST, etc.)
- Only a few experimental data for stopping power of hot matter (plasma) have been obtained.
- The production of a well-defined quasi-stable dense plasma target is difficult because of its high opacity and pressure.

- To describe the ion stopping in hot or warm dense matter, we are forced to rely on “theoretical” stopping power models applicable to a wide density-temperature range.

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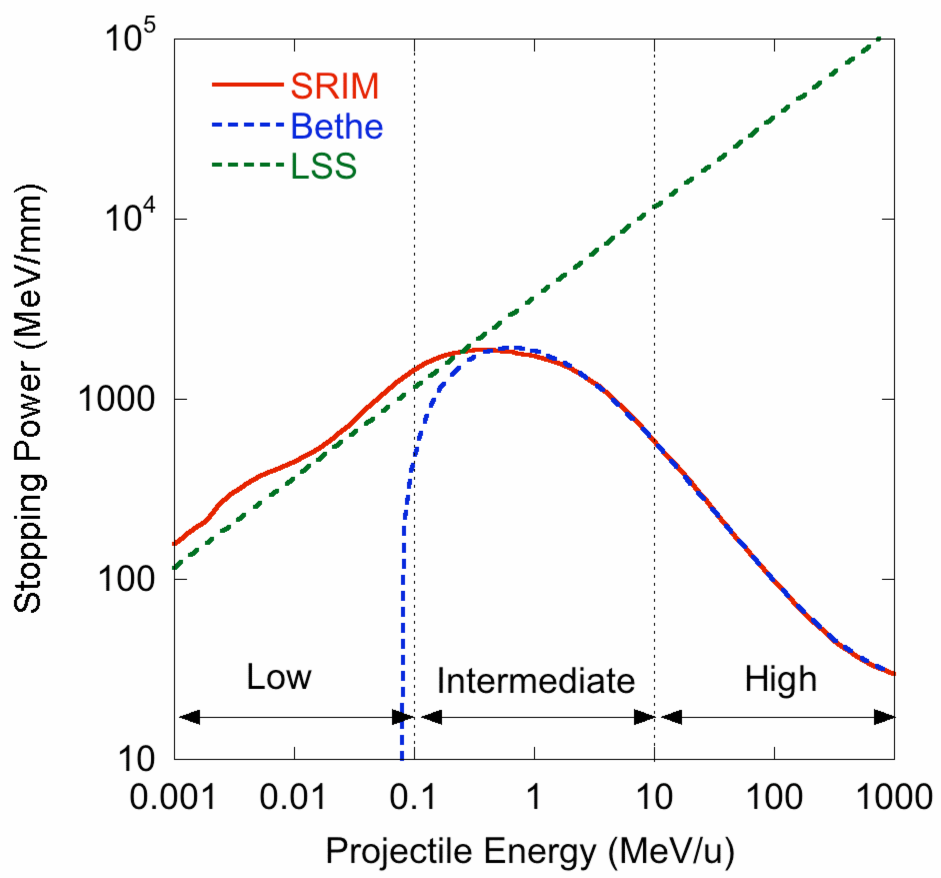
Electronic stopping is divided into three regimes.



- **Low-speed regime**
  - Lindhard-Scharff-Schiøtt (LSS) formula can roughly estimate dE/dx.

$$\boxed{S_e \propto v}$$

- **Intermediate-speed regime**
  - Bethe-type formula with effective charge can describe dE/dx.
- **High-speed regime**
  - Bethe-Bloch formula well explains dE/dx.

$$\boxed{S_e \propto (1/v^2)\ln(v^2)}$$

- Stopping power for projectiles with velocities more than 0.1 MeV/u (intermediate and high regimes) is important because it dominates the ion slowing process in a target.

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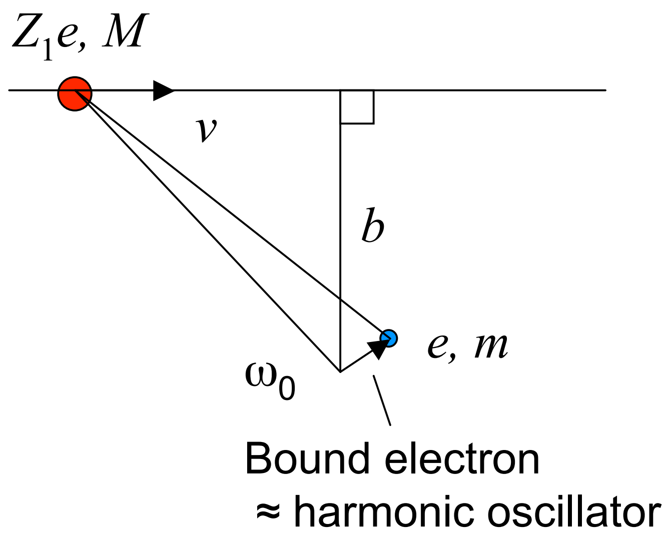
Bohr classical stopping formula

Energy transfer in dipole approximation:

$$\Delta E(b) = \frac{2(Z_1 e^2)^2}{mv^2}\left(\frac{1}{b^2}\right)\left[\xi^2 K_1^2(\xi) + \frac{1}{\gamma^2}\xi^2 K_0^2(\xi)\right]$$

$$\xi = \frac{\omega_0 b}{\gamma v}$$

Modified Bessel functions



Energy loss is calculated by integrating for all possible impact parameters *b*:

$$-\frac{dE}{dx} = NZ_2 \sum_j f_j \int_{b_{min}}^{\infty} \Delta E_j(b) \cdot 2\pi b\, db$$

$$= \frac{4\pi (ze^2)^2}{mv^2} NZ_2 L_{Bohr}$$

$$L_{Bohr} = \sum_j f_j \ln \frac{1.123 mv^3}{Z_1 e^2 \omega_j} - \ln(1-\beta^2) - \frac{\beta^2}{2}$$

f_j: oscillator strengh $\sum_j f_j = 1$

- Bohr formula gives good results for α particles and heavy ions with relatively low velocities.
- Quantum corrections are needed for light particles with higher velocities.

Stopping power formulae based on quantal perturbation theory.

- **Bethe formula:**

$$\boxed{\begin{aligned} L_{Bethe} &= \sum_j f_j \ln \frac{2mv^2}{\hbar\omega_j} - \ln(1-\beta^2) - \beta^2 \\ &= \ln \frac{2mv^2}{I} - \ln(1-\beta^2) - \beta^2 \end{aligned}}$$

I: Mean excitation energy $\ln I = \sum_j f_j \ln \hbar\omega_j$

- **Bloch formula:**

$$\boxed{\begin{aligned} \Delta L_{Bloch} &= \psi(1) - \mathrm{Re}\left\{\psi\left(1 + i\frac{Z_1 e^2}{\hbar v}\right)\right\} \\ L_{Bloch} &= L_{Bethe} + \Delta L_{Bloch} \end{aligned}}$$

$\psi(x)$: digamma function

Minimum impact parameter:

$b_{\min}^{(c)} = Z_1 e^2 / \gamma m v^2$ (classical)

$b_{\min}^{(q)} = \hbar / \gamma m v$ (quantal)

Bohr parameter:

$$\boxed{\eta = b_{\min}^{(c)} / b_{\min}^{(q)} = Z_1 e^2 / \hbar v}$$

$\eta > 1 \Rightarrow$ Bohr formula

$\eta \leq 1 \Rightarrow$ Bethe formula:

- Bloch formula gives Bethe formula at a high velocity limit and Bohr formula at a low velocity limit.

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Free electron gas model

- Excitation of conductive electrons in metal.
  - Individual excitation
  - Collective excitation (plasmon excitation)
- These excitations can be described with a dielectric response function in free electron gas $\varepsilon(k,\omega)$.
- The projectile is decelerated by an induced electric field and the stopping power is written by:

$$-\frac{dE}{dx}=\frac{4\pi(Z_1e^2)^2}{mv^2}\rho L_{FEG}, \qquad L_{FEG}(\rho,v)=\frac{i}{\pi\omega_p^2}\int_0^\infty\frac{dk}{k}\int_{-kv}^{kv}d\omega\omega\,\mathrm{Im}\left\{-\frac{1}{\varepsilon(k,\omega)}\right\}$$

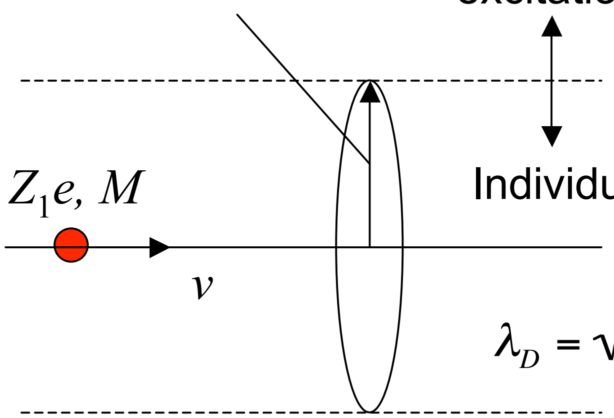
- Lindhard obtained a dielectric response function $\varepsilon(k,\omega)$ for zero-temperature electron gas.
- The free electron model can explain that the proportionality of dE/dx to v (projectile velocity) at $v < v_F$ (like LSS), and that to $(1/v^2)\ln(v^2)$ at $v > v_F$ (like Bethe formula), indicating that this model can be applied to almost all velocity ranges.

Local electron density model

- The free electron model is useful to describe the excitations of conductive electrons because…
  - it can treat the dynamic shielding effect,
  - it reproduces the dependency of dE/dx on projectile velocity from low-speed to high-speed regimes.
- However, for larger target one should take into account inner-shell electrons.
- The local electron density model uses electron density distribution function $\rho(\mathbf{r})$, which is determined by Hartree-like or Thomas-Fermi-like atomic model, instead of uniform electron density ρ used in the free electron gas model.

$$-\frac{dE}{dx} = \frac{4\pi(Z_1 e^2)^2}{mv^2} \int_0^\infty \rho(r) L_{FEG}(\rho, v) 4\pi r^2 dr$$

Stopping power of plasma free electrons



$$\lambda_D = \sqrt{4\pi n e^2 / m}$$

$$\left(-\frac{dE}{dx}\right)_{\text{free}} = \left(-\frac{dE}{dx}\right)_{\text{indiv}} + \left(-\frac{dE}{dx}\right)_{\text{coll}}$$

$$= \frac{4\pi (Z_1 e^2)^2}{m v^2} G(v / v_{th}) \ln\left(\frac{0.764 v}{b_{\min}\omega_p}\right)$$

$$G(x) = \operatorname{erf}(x/\sqrt{2}) - \sqrt{\pi/2}\, x \exp(-x^2/2)$$

$$b_{\min} = \min\{b_{\min}^{(c)}, b_{\min}^{(q)}\}$$

- Stopping power of plasma free electron can be naturally calculated by free electron gas model by using a plasma dielectric response function.
- Inside the Debye radius λ_D, the energy transfer is occurred by binary collisions between the projectile and the free electron.
- The projectile energy is transferred to free electrons outside the Debye radius via collective (plasmon) excitations.

For $v >> v_{th} = (kT/m)^{1/2}$

$$\left(-\frac{dE}{dx}\right)_{\text{free}} \approx \frac{4\pi (Z_1 e^2)^2}{m v^2} \ln\left(\frac{\gamma m v^3}{Z_1 e^2 \omega_p}\right)$$

Bohr formula with ω_p instead of $<\omega>$

Stopping power of partially ionized plasma

$$\left(-\frac{dE}{dx}\right)_{\text{plasma}} = \left(-\frac{dE}{dx}\right)_{\text{bound}} + \left(-\frac{dE}{dx}\right)_{\text{free}}$$

$$= \frac{4\pi(Z_1 e^2)^2}{mv^2} N\left\{(Z_2 - \bar{Z})\ln\Lambda_B + \bar{Z}G(v/v_{th})\ln\Lambda_F\right\}$$

$$\Lambda_B = \frac{2mv^2}{I}, \quad \Lambda_F = \frac{0.764v}{b_{\min}\omega_p}, \quad b_{\min} = \min\left[Z_1 e^2/mv^2, \hbar/mv\right]$$

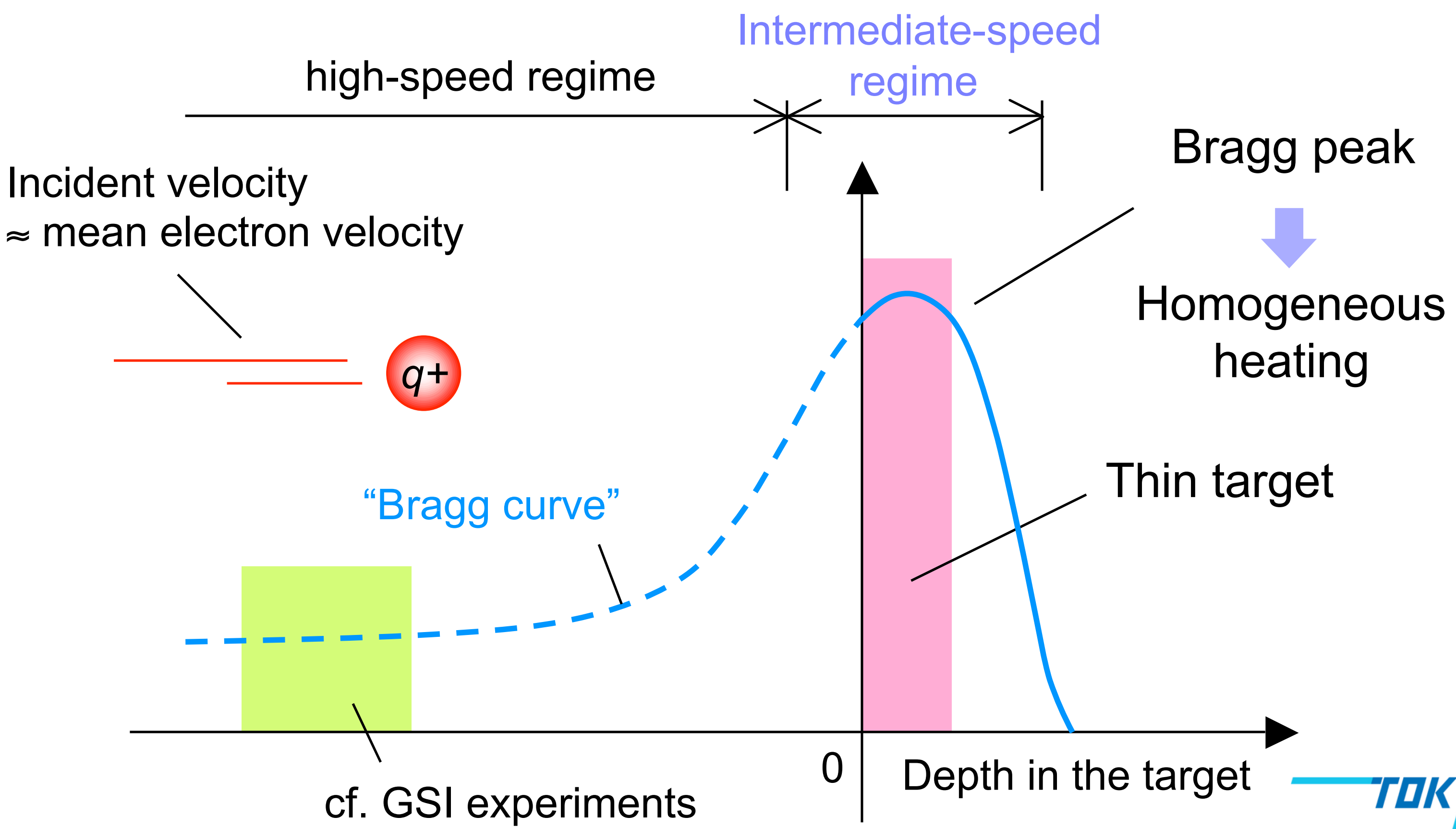
$$G(x) = \text{erf}(x/\sqrt{2}) - \sqrt{\pi/2}\,x\exp(-x^2/2)$$

Z_1 : projectile charge
Z_2 : target atomic number
m : electron mass
v : projectile velocity
v_{th}: electron thermal velocity
$\bar{Z}$: mean ion charge

- Free electrons and bound electrons are treated separately.
- To describe the stopping power of WDM, bound electrons and free electrons should be treated seamlessly with a unified stopping power model.

Pulsed heavy-ion beams are one of the options to produce “Warm Dense Matter (WDM)” in laboratories.

- Production of dense plasmas from a solid target by pulsed ion beams:
  - Thin target → Homogeneous and efficient heating using “Bragg peak”
  - ≈ 1 MeV/u heavy projectiles → Moderate cost



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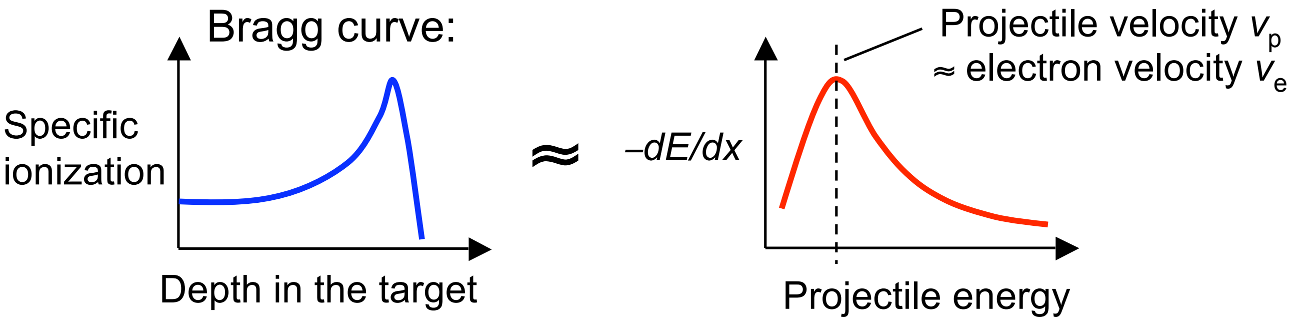
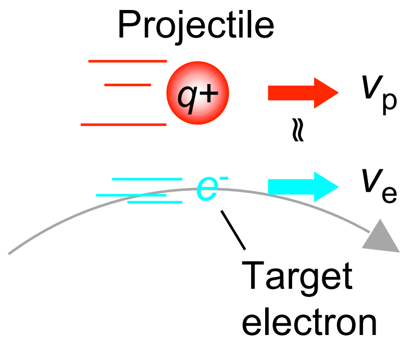
Change of Bragg-peak position / amplitude can induce unwanted perturbation to the scheduled hydro motion.

- Bragg curve ≈ $-dE/dx$ as a function of the projectile energy (reversed)

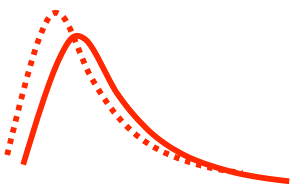


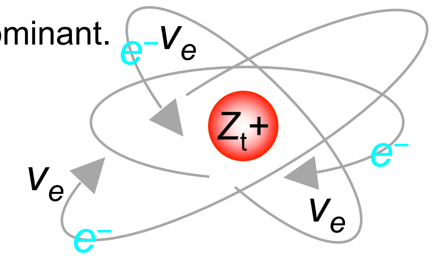


- Bound* / free electron velocity can change with target conditions:
  - Phase (gas, liquid, solid, plasma; atomic, molecular, crystal, ······)
  - Density, temperature

  → Bragg-peak position / height can also change!

*In WDM, contribution of bound electrons are dominant.





- Typical kinetic energy (velocity v_e) of electrons
  = typical potential energy (virial theorem)
  ≈ "mean excitation (ionization) energy I"

$$\therefore v_e \approx \sqrt{\frac{2I}{m_e}}$$

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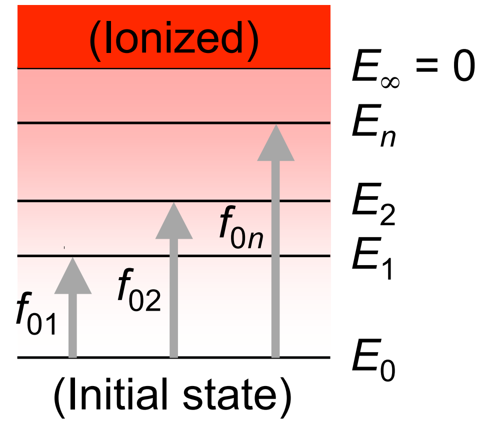
"Local plasma approximation" was applied to simply calculate the mean excitation energy *I*.

- Mean excitation energy I ≡ logarithmic mean of the excitation energy:

$$Z_{\mathrm{t}} \ln I = \sum_n f_{0n} \ln(E_n - E_0)$$

  - f_{0n}: Dipole oscillator strength for $0 \rightarrow n$ transition
  - Detailed data on the wave functions for all excited states are needed for calculation!



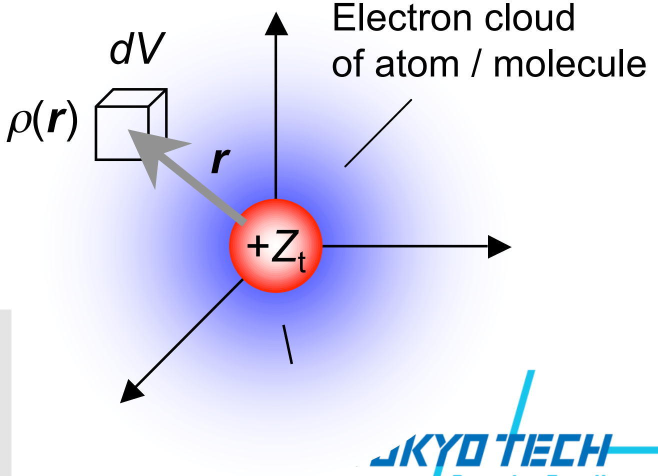
- Simple alternative: "Local plasma approximation":
  - Atom / molecule ≡ inhomogeneous electron gas
  - Local (position = $\boldsymbol{r}$) plasma frequency $\omega_{\mathrm{p}}(\boldsymbol{r})$
    → Dynamical response of the electron cloud

$$\omega_{\mathrm{p}}(\mathbf{r}) = \sqrt{\frac{e^2 \rho(\mathbf{r})}{\varepsilon_0 m_e}} \quad \leftrightarrow \quad \text{Plasmon energy } \hbar\omega_{\mathrm{p}}(\boldsymbol{r})$$

  - Excitation energy ≈ local plasmon energy

$$Z_t \ln I = \int \rho(\mathbf{r}) \ln\left(\hbar\omega_p(\mathbf{r})\right) dV$$

Electron density distribution ρ(r) must be determined



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To take into account the target electron motion, dE/dt was calculated based on a classical collision theory for two moving charged particles.

- Differential scattering cross section for isotropic electron velocity distribution:

$$\frac{d\sigma}{d(\Delta E)} = \frac{\pi}{3}\frac{(Z_1 e^2)^2}{v^2} \times F$$

ΔE: Energy transfer to one electron

$$\begin{aligned} F &\equiv 3v_e'^2 - v_e^2 \quad \text{for } 0 < \delta E \le \delta E^* \\ &\equiv \frac{(v'+v)^3 + (v_e' - v_e)^3}{2v_e} \quad \text{for } \delta E^* \le \delta E < \delta E_{\max} \\ &\equiv 0 \quad \text{for all other cases} \end{aligned}$$

$$\left(v_e = \sqrt{\frac{2I}{m_e}}, \quad v' \equiv \sqrt{v^2 - \frac{2\Delta E}{M}}, \quad v_e' \equiv \sqrt{v_e^2 + \frac{2\Delta E}{m_e}}, \quad \Delta E_{\max} \equiv 2mv(v+v_e), \quad \Delta E^* \equiv 2m_e v(v - v_e) \right)$$

- Projectile charge q was roughly estimated by a simple Thomas-Fermi scaling:

$$Z_{eff} = Z_1\left\{1 - \exp\left(-\frac{v}{Z_1^{2/3} v_{\mathrm{B}}}\right)\right\}$$

- Stopping cross section S can be calculated by integrating $d\sigma/d(\Delta E)$ over all possible energy transfer:

$$\boxed{S_e = Z_2 \int_{\delta E_{min}}^{\delta E_{\max}} \Delta E \frac{d\sigma}{d(\Delta E)} d(\Delta E)}$$

Minimum $\Delta E = I$

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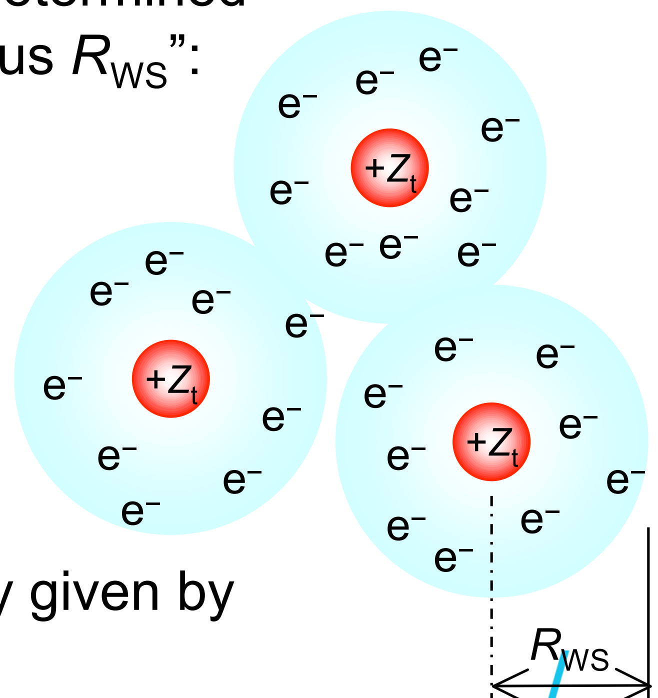
A finite temperature Thomas-Fermi model was used to obtain electron density function $\rho(\mathbf{r})$.

- Phase-space (r, p) distribution of electrons around a nucleus:

$$f_{\mathrm{e}}(r,p) = \frac{1}{\pi^2\hbar^3}\frac{p^2}{1+\exp\left(\dfrac{p^2/2m - eV(r) - E_{\mathrm{F}}}{kT}\right)}$$

- Fermi energy E_{F} (chemical potential μ) was determined by the neutrality within the "Wigner-Seitz radius R_{WS}":

$$\int_0^{R_{\mathrm{WS}}} \rho(r)dr^3 = Z_{\mathrm{t}}, \quad R_{\mathrm{WS}} \equiv \sqrt[3]{\frac{3n_{\mathrm{atom}}}{4\pi}}$$



- Electrostatic potential $V(r)$:

$$V(r) = \frac{1}{4\pi\varepsilon_0}\left(\frac{Z_{\mathrm{t}}e}{r} - \int_V \frac{e\rho(r')}{|r-r'|}dr'^3\right)$$

- The electron density distribution is recursively given by

$$\rho(r) = \int_0^{\infty} f_{\mathrm{e}}(r,p)dp.$$

By partially integrating $f_e(r,p)$, distributions of bound- and free electrons were separately calculated.

- Bound-electron component:

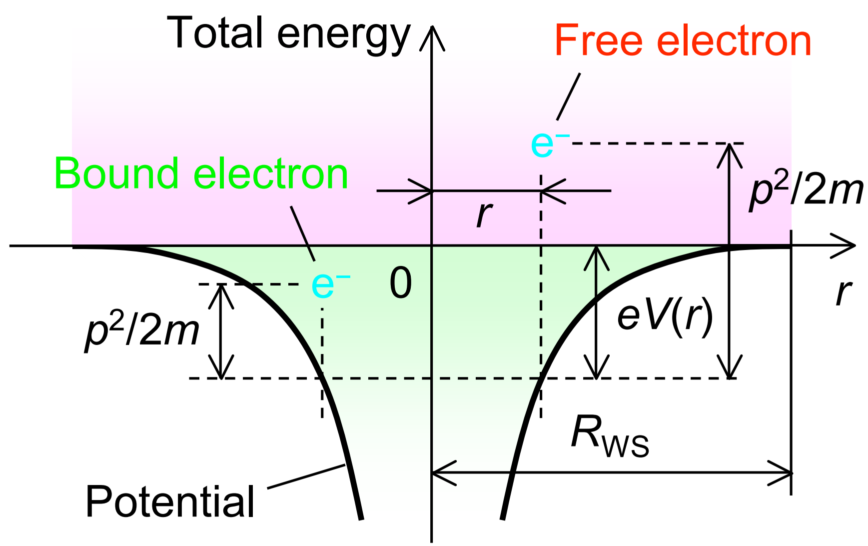
$$\rho_b(r) = \int_0^{\sqrt{2meV(r)}} f_e(r,p)dp$$

$$v_{eb}(r) = \frac{1}{m}\left(\int_0^{\sqrt{2meV(r)}} p^2 f_e(r,p)dp\right)^{1/2}$$

- Free-electron component:

$$\rho_f(r) = \int_{\sqrt{2meV(r)}}^{\infty} f_e(r,p)dp$$

$$v_{ef}(r) = \frac{1}{m}\left(\int_{\sqrt{2meV(r)}}^{\infty} p^2 f_e(r,p)dp\right)^{1/2}$$

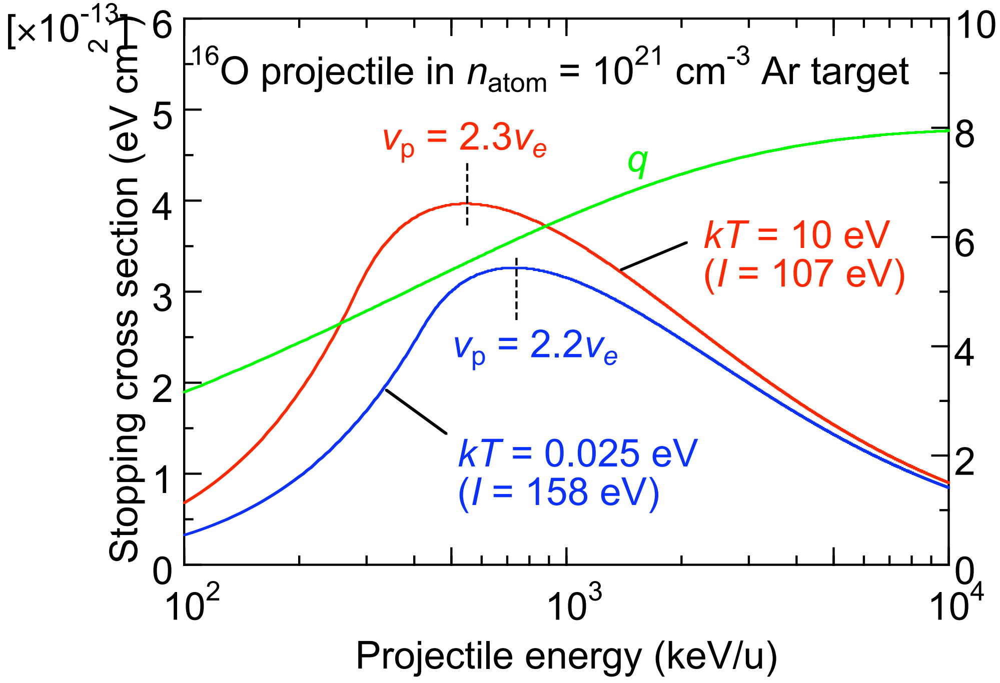


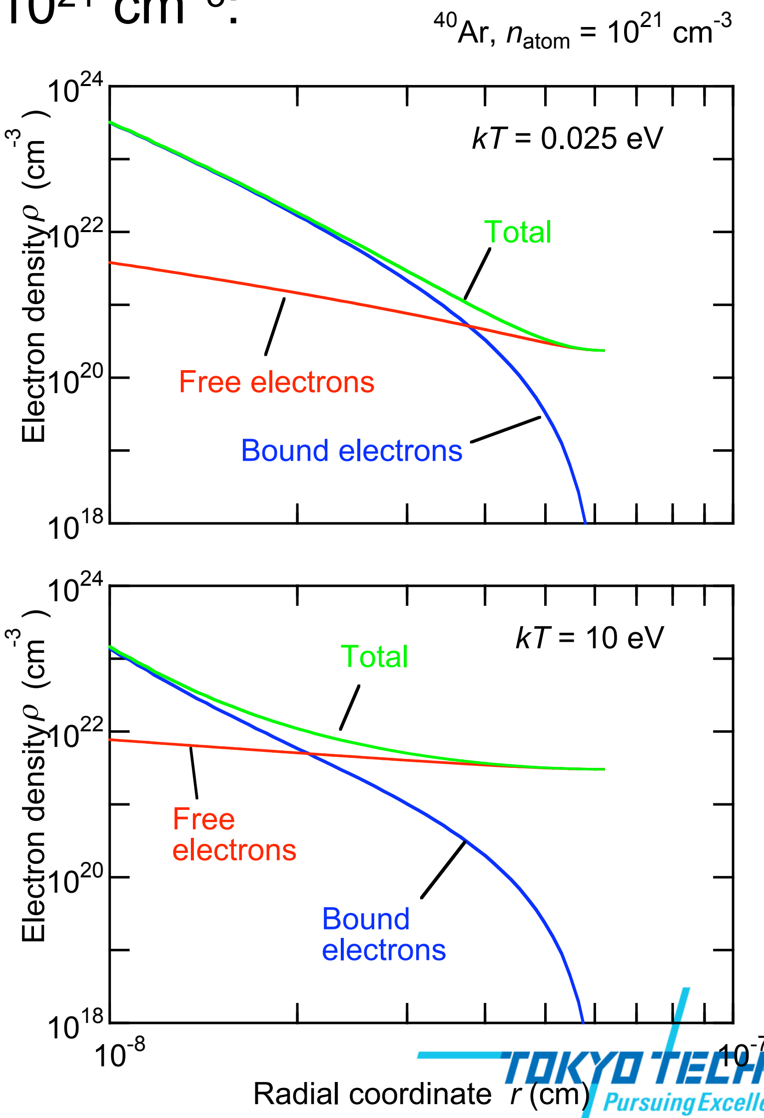
- These integrals were evaluated analytically in part, using tables of complete- and incomplete Fermi-Dirac integrals:

$$F_j(x) \equiv \int_0^{\infty} \frac{y^j dy}{1+e^{y-x}}, \quad F_j(x;\beta) \equiv \int_{\beta}^{\infty} \frac{y^j dy}{1+e^{y-x}}$$

When the target is heated, the Bragg peak moves deeper inside the target, and the stopping is enhanced.

- Temperature-dependence of $\rho(\mathbf{r})$ at $n_{atom} = 10^{21}$ cm^{-3}:
  - Even at the room temperature, weak pressure ionization is observed.
  - For high kT, bound electron density in the outer shell decreases by thermal ionization.
- Behavior of $-dE/dx$ for fixed density:





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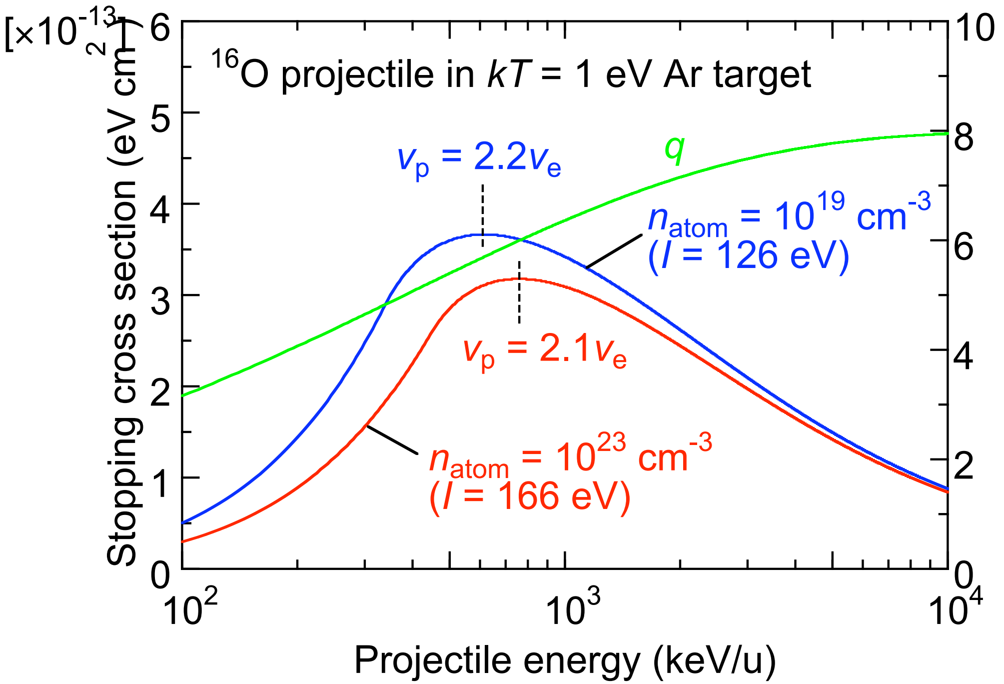
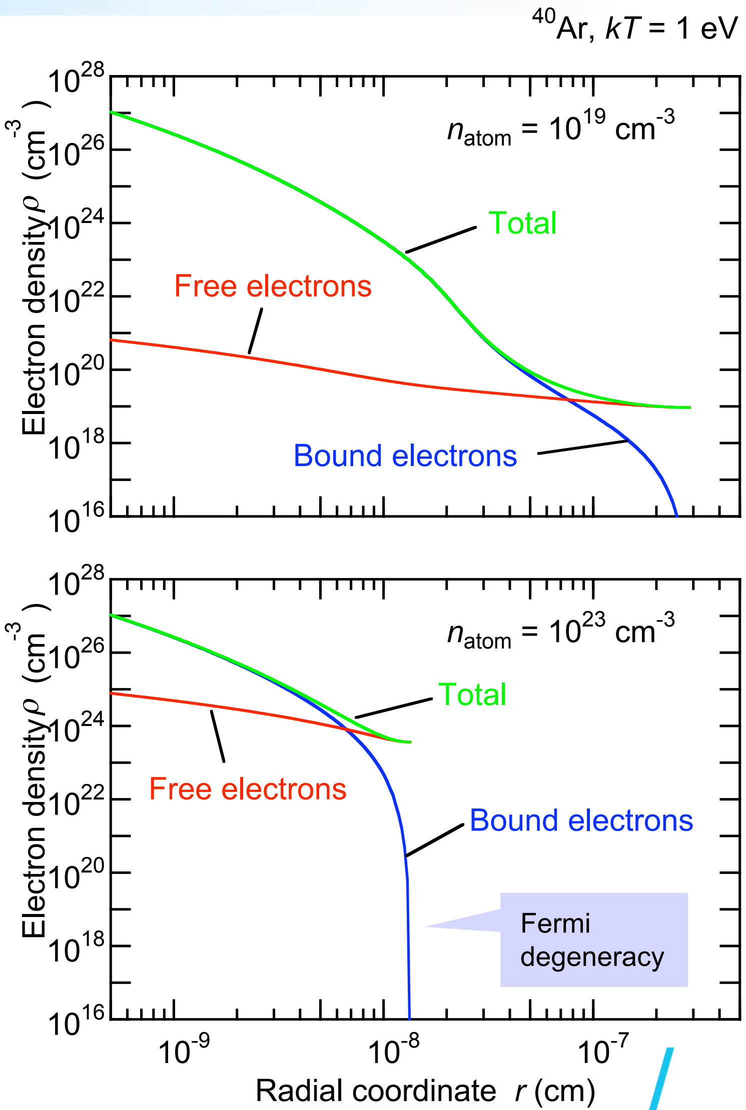
When the target expands, similar effects are expected for the Bragg-peak position / height.

- Density-dependence of $\rho(\boldsymbol{r})$ at kT =1 eV:
  - For low densities, we see a core part and a peripheral thermal part.
  - For high densities, the thermal part is compressed into the core part.
- Behavior of $-dE/dx$ for fixed temperature:





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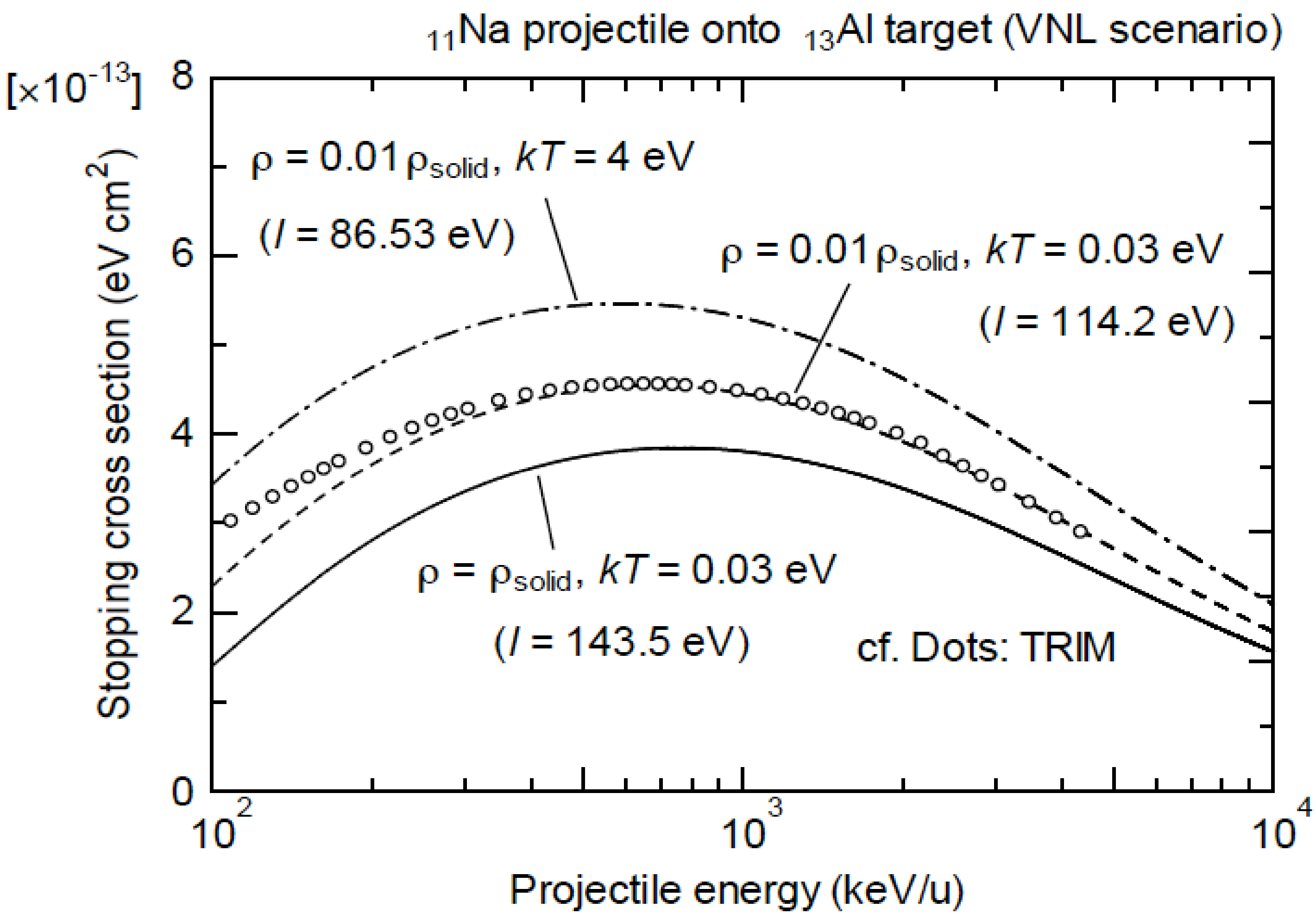
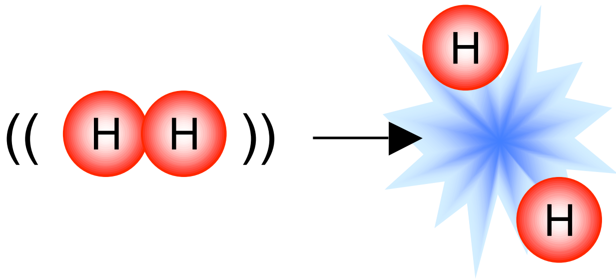
The developed stopping power model almost reproduced SRIM stopping power data.



As a simplest phase transition of the target matter, dissociation of hydrogen molecule was investigated.

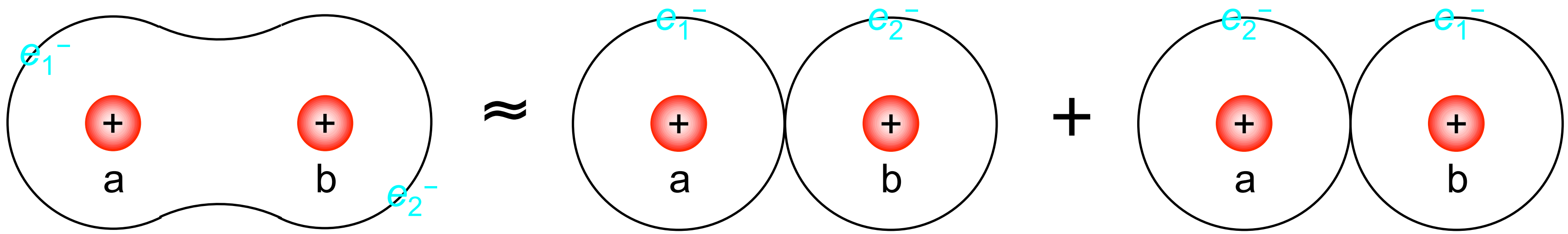
- Electron density distribution in a hydrogen molecule H_2 was calculated using a valence-bond (VB) type approximated wave function.
  - 1s-atomic wave function (ground state)

$$\psi(\mathbf{r}) = (1s) = \frac{1}{\sqrt{\pi} a_0^{3/2}} \exp\left(-\frac{r}{a_0}\right)$$



  - "Heitler-London" type molecular wave function:

$$\Psi(\mathbf{r}_1,\mathbf{r}_2) = A\left(\psi_a(r_1)\psi_b(r_2) + \psi_a(r_2)\psi_b(r_1)\right) \qquad \left(A \equiv \frac{1}{\int \Psi^* \Psi \, dV} \right)$$



  - Electron density distribution:

$$\rho(r) = \rho(r_1) + \rho(r_2) = \int \Psi(r_1,r_2)^* \Psi(r_1,r_2) dV_2 + \int \Psi(r_1,r_2)^* \Psi(r_1,r_2) dV_1$$

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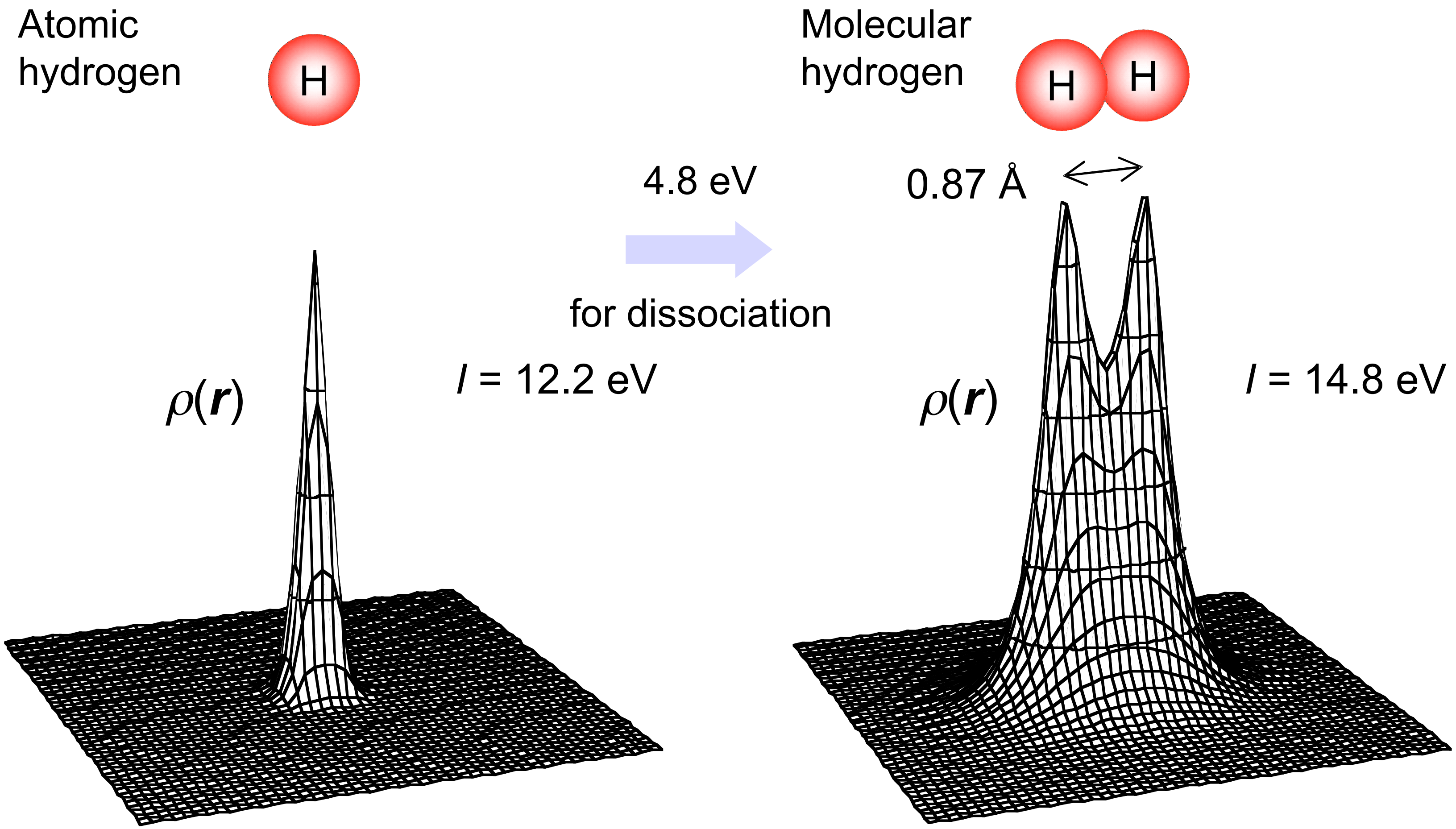
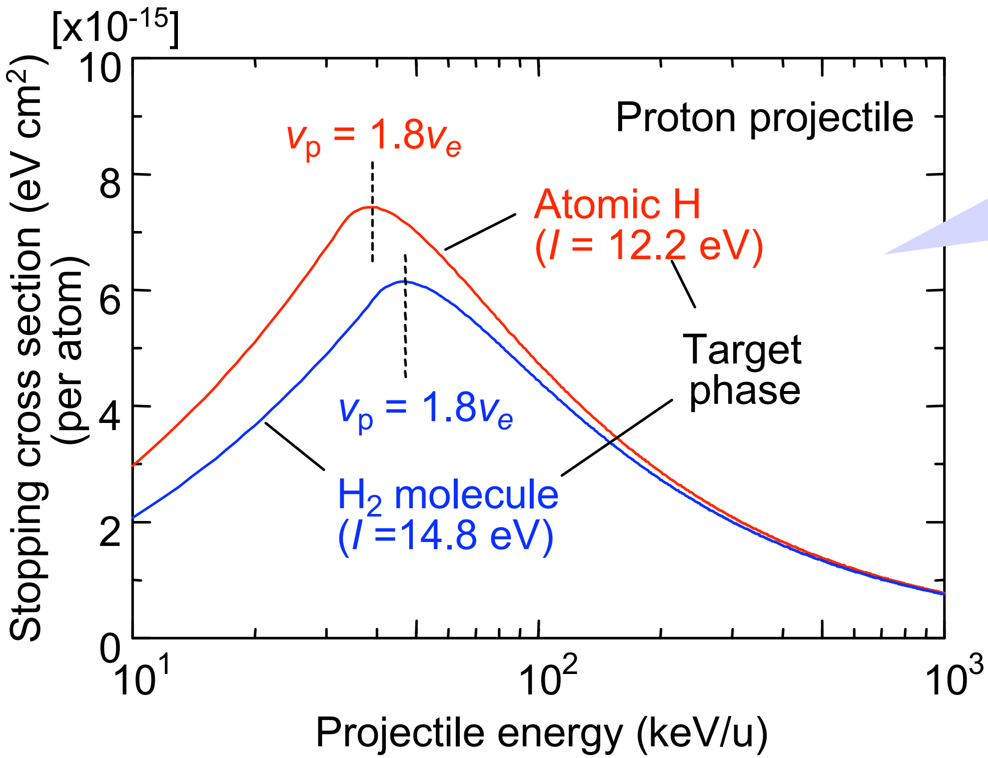
By using the electron distribution, mean excitation energies of H and H_2 were evaluated.

- Electron density distribution $\rho(\boldsymbol{r})$ and evaluated mean excitation energies I per atom:



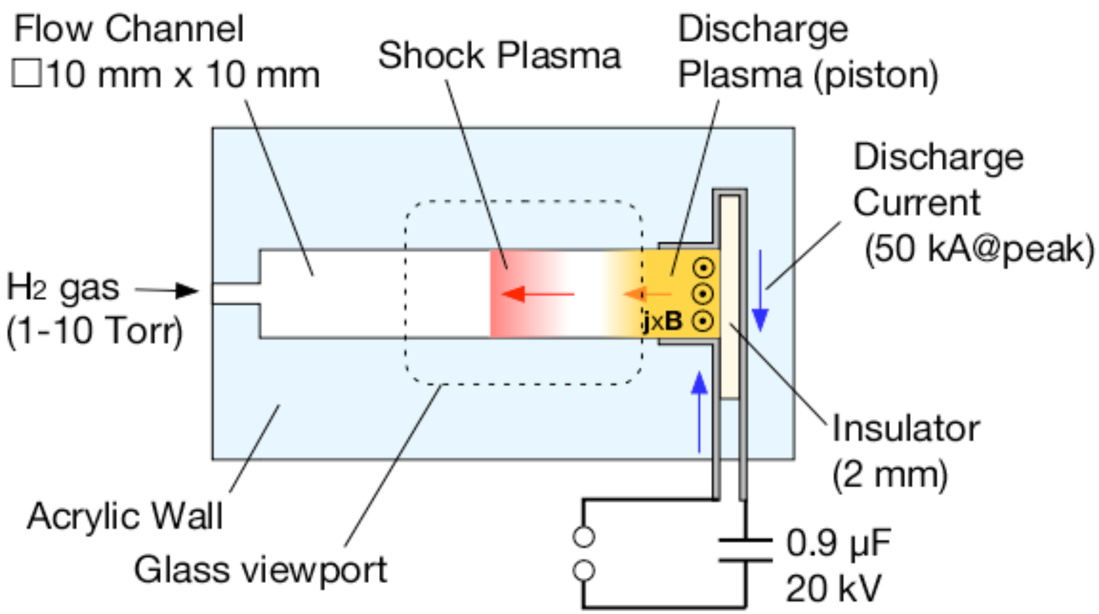
Bragg-peak position / height can be influenced by dissociation of molecules.

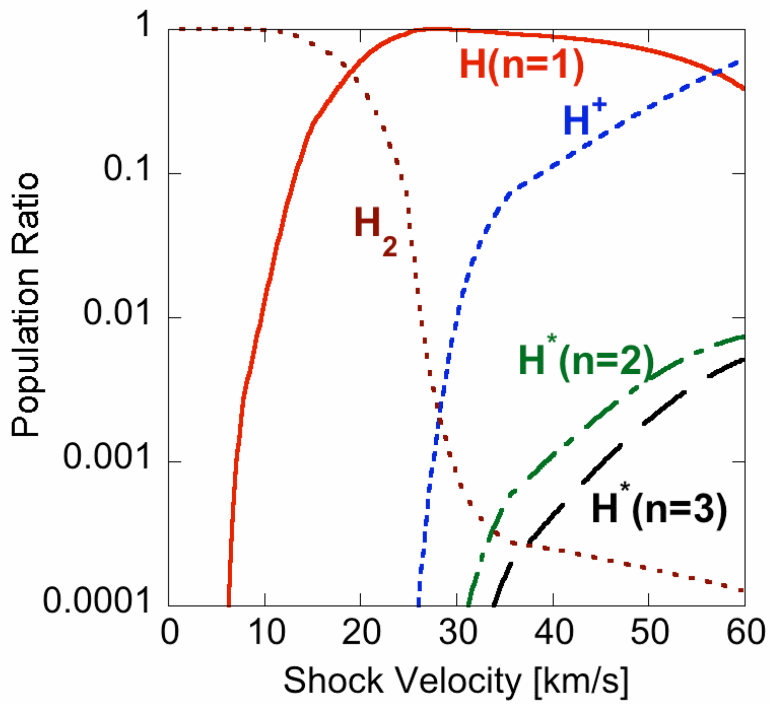
- Stopping cross section (per atom) for molecular and atomic hydrogen targets:
  - $Z_{eff}=Z_1=1$ (proton) is assumed for all projectile energies.
  - Bragg-peak is observed at $v_p \approx 2v_e$, owing to isotropic motion of target electrons.



Effects of excited states have not yet been taken into account.

An electromagnetically driven shock tube was developed for beam-plasma interaction experiments.





- A strong shock wave was driven by the piston discharge plasma accelerated by **jxB** force.
- The parameters of the shock-produced plasma can be controlled by shock velocity and easily predicted by Rankin-Hugoniot relation.
- Warm hydrogen plasma will be used for benchmark experiments.

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Summary

- To calculate the stopping power of warm dense matter in a projectile velocity range around the Bragg-peak energy, a simple model based on a classical collision stopping theory with a finite-temperature Thomas-Fermi statistical model.

- Bragg-peak position / height can change with the target conditions, such as the density, temperature and the chemical phase.

- Concerning the production of WDM by pulsed ~MeV/u heavy ion beams, the above effect might influence the quality of WDM, owing to perturbations of the energy-deposition profile and hydro motion of the heated matter.

- A electromagnetically-driven shock tube was developed to perform benchmark experiments for stopping-power models.

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